Linear Discriminant Analysis

Nate Wells

Math 243: Stat Learning

November 3rd, 2021

Outline

In today's class, we will...

- Discuss LDA theory and motivation
- Build an LDA classifier by hand

Section 1

LDA

Recall that for a binary classification problem, the average test error rate is minimized using the Bayes' classifier:

$$f(x_0) = \operatorname{argmax}_j P(Y = j | X = x_0) \quad j \in \{0, 1\}$$

Recall that for a binary classification problem, the average test error rate is minimized using the Bayes' classifier:

$$f(x_0) = \operatorname{argmax}_j P(Y = j | X = x_0) \quad j \in \{0, 1\}$$

Both KNN and Logistic regression attempt to estimate the conditional probability p(X) = P(Y = 1 | X):

Recall that for a binary classification problem, the average test error rate is minimized using the Bayes' classifier:

$$f(x_0) = \operatorname{argmax}_j P(Y = j | X = x_0) \ j \in \{0, 1\}$$

Both KNN and Logistic regression attempt to estimate the conditional probability p(X) = P(Y = 1 | X):

• Logistic regression:

$$p(X) = \frac{e^{\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p}}{1 + e^{\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p}}$$

Recall that for a binary classification problem, the average test error rate is minimized using the Bayes' classifier:

$$f(x_0) = \operatorname{argmax}_j P(Y = j | X = x_0) \ j \in \{0, 1\}$$

Both KNN and Logistic regression attempt to estimate the conditional probability p(X) = P(Y = 1 | X):

• Logistic regression:

$$p(X) = \frac{e^{\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p}}{1 + e^{\beta_0 + \beta_1 X_1 + \dots + \beta_p X_p}}$$

• KNN:

$$p(X) = \frac{1}{K} \sum_{i \in N_0} I(y_i = 1)$$

The Law of Total Probability

Suppose A_1, A_2, \ldots, A_k are a list of events that are:

- mutually exclusive: $P(A_i \text{ and } A_j) = 0$
- exhaustive: $P(A_1) + P(A_2) \cdots + P(A_k) = 1$
 - Example: Flip two coins, and let A_1 = both flips are different, A_2 = both flips are heads, A_3 = both flips are tails.

Then for any other event B,

 $P(B) = P(B|A_1)P(A_1) + P(B|A_2)P(A_2) + \dots + P(B|A_k)P(A_k)$

The Law of Total Probability

Suppose A_1, A_2, \ldots, A_k are a list of events that are:

- mutually exclusive: $P(A_i \text{ and } A_j) = 0$
- exhaustive: $P(A_1) + P(A_2) \cdots + P(A_k) = 1$
 - Example: Flip two coins, and let A_1 = both flips are different, A_2 = both flips are heads, A_3 = both flips are tails.

Then for any other event B,

 $P(B) = P(B|A_1)P(A_1) + P(B|A_2)P(A_2) + \dots + P(B|A_k)P(A_k)$

Example

Consider two boxes of marbles, the first containing 60% blue and 40% red, and the second containing 10% blue and 90% red. Suppose we draw a marble from the first box with 20% probability and from the second box with 80% probability.

• What is the probability we draw a blue marble?

Bayes' Rule

For any events A and B,

$$P(A|B) = rac{P(B|A)P(A)}{P(B)}$$

Bayes' Rule

For any events A and B,

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

- *P*(*A*) is called the *prior probability* of *A* and represents our initial beliefs about the event *A*.
- Suppose *B* is an event that we observe occurring.
- P(A|B) is called the *posterior probability* of A and represents our updated beliefs about the event A in light of the event B.

Bayes' Rule

For any events A and B,

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

- *P*(*A*) is called the *prior probability* of *A* and represents our initial beliefs about the event *A*.
- Suppose *B* is an event that we observe occurring.
- *P*(*A*|*B*) is called the *posterior probability* of *A* and represents our updated beliefs about the event *A* in light of the event *B*.

Example

Suppose a test for a certain disease has specificity .8 and sensitivity .95, and that the disease has prior prevalence of 0.01. Find the posterior probability that an individual who tests positive for the disease actually has the disease.

For classification problems, we want to know $P(Y = A_j | X = x_0)$.

For classification problems, we want to know $P(Y = A_j | X = x_0)$.

• Using Bayes' Rule:

$$P(Y = A_j | X = x_0) = \frac{P(X = x_0 | Y = A_j)P(Y = A_j)}{P(X = X_0)}$$
$$= \frac{P(X = x_0 | Y = A_j)P(Y = A_j)}{\sum_i P(X = X_0 | Y = A_i)P(Y = A_i)}$$

For classification problems, we want to know $P(Y = A_j | X = x_0)$.

• Using Bayes' Rule:

$$P(Y = A_j | X = x_0) = \frac{P(X = x_0 | Y = A_j)P(Y = A_j)}{P(X = X_0)}$$
$$= \frac{P(X = x_0 | Y = A_j)P(Y = A_j)}{\sum_i P(X = X_0 | Y = A_i)P(Y = A_i)}$$

- We estimate the conditional probability of the response using...
 - The conditional distribution $P(X = x_0 | Y = A_j)$ of each predictor given the response
 - The prior distribution $\pi_i = P(Y = A_i)$ of the response

For classification problems, we want to know $P(Y = A_j | X = x_0)$.

• Using Bayes' Rule:

$$P(Y = A_j | X = x_0) = \frac{P(X = x_0 | Y = A_j)P(Y = A_j)}{P(X = X_0)}$$
$$= \frac{P(X = x_0 | Y = A_j)P(Y = A_j)}{\sum_i P(X = X_0 | Y = A_i)P(Y = A_i)}$$

- We estimate the conditional probability of the response using...
 - The conditional distribution $P(X = x_0 | Y = A_i)$ of each predictor given the response
 - The prior distribution $\pi_i = P(Y = A_i)$ of the response
- In practice, we don't have access to the conditional distributions of the predictors, so need to estimate them based on data.



• Suppose we have just one predictor X and a multi-level categorical response Y.

- Suppose we have just one predictor X and a multi-level categorical response Y.
- What is the most "natural" assumption for the conditional distribution of X, given $Y = A_j$?

- Suppose we have just one predictor X and a multi-level categorical response Y.
- What is the most "natural" assumption for the conditional distribution of X, given $Y = A_j$?
- If X is normal with mean μ_j and variance σ_i^2 , its density is

$$P(X = x | Y = A_j) = f_j(x) = \frac{1}{\sqrt{2\pi\sigma_j^2}}e^{-(x-\mu_j)^2/2\sigma_j^2}$$

- Suppose we have just one predictor X and a multi-level categorical response Y.
- What is the most "natural" assumption for the conditional distribution of X, given $Y = A_j$?
- If X is normal with mean μ_j and variance σ_j^2 , its density is

$$P(X = x | Y = A_j) = f_j(x) = \frac{1}{\sqrt{2\pi\sigma_j^2}}e^{-(x-\mu_j)^2/2\sigma_j^2}$$

• Moreover, if we assume all conditional distributions have the same variance $\sigma_j^2 = \sigma^2$, we can simplify our model.

Likelihood Ratio

• To determine to which class an observation belongs, based on the conditional distribution of predictors, we consider the likelihood ratio (LR):

$$LR = \frac{P(Y = A_j | X = x_0)}{P(Y = A_k | X = x_0)}$$

Likelihood Ratio

• To determine to which class an observation belongs, based on the conditional distribution of predictors, we consider the likelihood ratio (LR):

$$LR = \frac{P(Y = A_j | X = x_0)}{P(Y = A_k | X = x_0)}$$

• If $LLR \ge 1$, we should predict A_j over A_k . Otherwise, predict A_k over A_j .

Likelihood Ratio

 To determine to which class an observation belongs, based on the conditional distribution of predictors, we consider the likelihood ratio (LR):

$$LR = \frac{P(Y = A_j | X = x_0)}{P(Y = A_k | X = x_0)}$$

- If LLR ≥ 1 , we should predict A_j over A_k . Otherwise, predict A_k over A_j .
- And using Bayes' Rule:

$$\frac{P(Y = A_j | X = x_0)}{P(Y = A_k | X = x_0)} = \frac{P(X = x_0 | Y = A_j)P(Y = A_j)/P(X = x_0)}{P(X = x_0 | Y = A_k)P(Y = A_k)/P(X = x_0)}$$
$$= \frac{P(X = x_0 | Y = A_j)P(Y = A_j)}{P(X = x_0 | Y = A_k)P(Y = A_k)}$$
$$= \frac{e^{-(x_0 - \mu_j)^2/2\sigma^2} \pi_j}{e^{-(x_0 - \mu_k)^2/2\sigma^2} \pi_k}$$

The Log-liklihood Ratio

The log-liklihood ratio is obtained by taking natural log of the liklihood ratio:

$$\ln \text{LR} = \ln \frac{P(Y = A_j | X = x_0)}{P(Y = A_k | X = x_0)}$$
$$= \ln \frac{e^{-(x_0 - \mu_j)^2 / 2\sigma^2} \pi_j}{e^{-(x_0 - \mu_k)^2 / 2\sigma^2} \pi_k}$$
$$= (x_0 - \mu_k)^2 / 2\sigma^2 - (x_0 - \mu_j)^2 / 2\sigma^2 + \ln \pi_j - \ln \pi_k$$

The Log-liklihood Ratio

The log-liklihood ratio is obtained by taking natural log of the liklihood ratio:

$$\ln \text{LR} = \ln \frac{P(Y = A_j | X = x_0)}{P(Y = A_k | X = x_0)}$$
$$= \ln \frac{e^{-(x_0 - \mu_j)^2 / 2\sigma^2} \pi_j}{e^{-(x_0 - \mu_k)^2 / 2\sigma^2} \pi_k}$$
$$= (x_0 - \mu_k)^2 / 2\sigma^2 - (x_0 - \mu_j)^2 / 2\sigma^2 + \ln \pi_j - \ln \pi_k$$

• The decision boundary between A_j and A_k is the point c where $\ln LR = 0$, or

$$(c - \mu_k)^2 / 2\sigma^2 + \ln \pi_j = (c - \mu_j)^2 / 2\sigma^2 + \ln \pi_k$$

The Log-liklihood Ratio

The log-liklihood ratio is obtained by taking natural log of the liklihood ratio:

$$\ln \text{LR} = \ln \frac{P(Y = A_j | X = x_0)}{P(Y = A_k | X = x_0)}$$
$$= \ln \frac{e^{-(x_0 - \mu_j)^2 / 2\sigma^2} \pi_j}{e^{-(x_0 - \mu_k)^2 / 2\sigma^2} \pi_k}$$
$$= (x_0 - \mu_k)^2 / 2\sigma^2 - (x_0 - \mu_j)^2 / 2\sigma^2 + \ln \pi_j - \ln \pi_k$$

• The decision boundary between A_j and A_k is the point c where $\ln LR = 0$, or

$$(c - \mu_k)^2 / 2\sigma^2 + \ln \pi_j = (c - \mu_j)^2 / 2\sigma^2 + \ln \pi_k$$

Solving for c gives

$$c = rac{\mu_1 + \mu_2}{2} + rac{\sigma^2 (\ln \pi_k - \ln \pi_j)}{\mu_j - \mu_k}$$

Binary Classfication with Uniform Prior

Suppose Y is binary, and that each of X|Y = 0 and X|Y = 1 are Normal with common variance σ and means μ_0 and μ_1 . Moreover, assume a uniform prior $\pi_0 = \pi_1 = \frac{1}{2}$

Binary Classfication with Uniform Prior

Suppose Y is binary, and that each of X|Y = 0 and X|Y = 1 are Normal with common variance σ and means μ_0 and μ_1 . Moreover, assume a uniform prior $\pi_0 = \pi_1 = \frac{1}{2}$ Solve for c in

$$(c - \mu_k)^2 / 2\sigma^2 + \ln \pi_j = (c - \mu_j)^2 / 2\sigma^2 + \ln \pi_k$$

Binary Classfication with Uniform Prior

Suppose Y is binary, and that each of X|Y = 0 and X|Y = 1 are Normal with common variance σ and means μ_0 and μ_1 . Moreover, assume a uniform prior $\pi_0 = \pi_1 = \frac{1}{2}$ Solve for c in

$$(c - \mu_k)^2 / 2\sigma^2 + \ln \pi_j = (c - \mu_j)^2 / 2\sigma^2 + \ln \pi_k$$

We get
$$c = \frac{\mu_1 + \mu_2}{2}$$

Plots

Suppose $X|Y = 0 \sim N(0,1)$ and $X|Y = 1 \sim N(4,1)$



If we ${\bf knew}$ the conditional distribution of the predictors, we could easily create decision boundaries.

• But we only have data, so we need to estimate those distributions.

- But we only have data, so we need to estimate those distributions.
- A normal distribution requires only 2 parameters: μ and σ .

- But we only have data, so we need to estimate those distributions.
- A normal distribution requires only 2 parameters: μ and σ .
 - We need one estimate of μ for each level of Y.
 - Since we assumed each conditional distribution had the same variance, we need only 1 estimate for σ

- But we only have data, so we need to estimate those distributions.
- A normal distribution requires only 2 parameters: μ and σ .
 - We need one estimate of μ for each level of Y.
 - Since we assumed each conditional distribution had the same variance, we need only 1 estimate for σ
- LDA is an algorithm for obtaining these estimates and then classifying based on log-likelihood ratio.

- But we only have data, so we need to estimate those distributions.
- A normal distribution requires only 2 parameters: μ and σ .
 - We need one estimate of μ for each level of Y.
 - Since we assumed each conditional distribution had the same variance, we need only 1 estimate for σ
- LDA is an algorithm for obtaining these estimates and then classifying based on log-likelihood ratio.
- Our estimates for μ_j and σ^2 are:

$$\hat{\mu}_j = \frac{1}{n_j} \sum_{i:y_i = A_j} x_i \qquad \hat{\sigma}^2 = \frac{1}{n - \ell} \sum_{j=1}^{\ell} \sum_{i:y_i = A_j} (x_i - \hat{\mu}_j)^2$$

$$\delta_j(x) = x \cdot rac{\mu_j}{\sigma^2} - rac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

Rather than comparing log likelihoods, we could instead look at the log conditional probability for each level. This function $\delta_j(x)$ is called the *discriminant* for level *j*:

$$\delta_j(x) = x \cdot rac{\mu_j}{\sigma^2} - rac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

• The discriminant is obtained by taking log-probabilities and discarding terms in the sum that don't depend on *j*.

$$\delta_j(x) = x \cdot rac{\mu_j}{\sigma^2} - rac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

- The discriminant is obtained by taking log-probabilities and discarding terms in the sum that don't depend on *j*.
- We can then assign an observation x_0 to the class whose discriminant is largest at $x = x_0$.

$$\delta_j(x) = x \cdot rac{\mu_j}{\sigma^2} - rac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

- The discriminant is obtained by taking log-probabilities and discarding terms in the sum that don't depend on *j*.
- We can then assign an observation x_0 to the class whose discriminant is largest at $x = x_0$.
- Why is LDA called Linear Discriminant Analysis?

$$\delta_j(x) = x \cdot \frac{\mu_j}{\sigma^2} - \frac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

- The discriminant is obtained by taking log-probabilities and discarding terms in the sum that don't depend on *j*.
- We can then assign an observation x_0 to the class whose discriminant is largest at $x = x_0$.
- Why is LDA called Linear Discriminant Analysis?
 - Because the discriminant function is linear in x.

$$\delta_j(x) = x \cdot rac{\mu_j}{\sigma^2} - rac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

- The discriminant is obtained by taking log-probabilities and discarding terms in the sum that don't depend on *j*.
- We can then assign an observation x_0 to the class whose discriminant is largest at $x = x_0$.
- Why is LDA called Linear Discriminant Analysis?
 - Because the discriminant function is linear in x.
 - Using this classification algorithm will result in linear decision boundaries.

Section 2

Handmade LDA model

Suppose Y is a categorical variable with ℓ levels, and for each level A_j , that

```
X|Y = A_j \sim N(\mu_j, \sigma).
```

Suppose Y is a categorical variable with ℓ levels, and for each level A_j , that

$$X|Y = A_j \sim N(\mu_j, \sigma).$$

The discriminant function

$$\delta_j(x) = x \cdot rac{\mu_j}{\sigma^2} - rac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

can be used to classify an observation by choosing the level A_j whose discriminant is largest at x.

Suppose Y is a categorical variable with ℓ levels, and for each level A_j , that

$$X|Y = A_j \sim N(\mu_j, \sigma).$$

The discriminant function

$$\delta_j(x) = x \cdot \frac{\mu_j}{\sigma^2} - \frac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

can be used to classify an observation by choosing the level A_j whose discriminant is largest at x.

We estimate the values of μ_i and σ from the sample data:

$$\hat{\mu}_j = \frac{1}{n_j} \sum_{i: y_i = A_k} x_i$$

Suppose Y is a categorical variable with ℓ levels, and for each level A_j , that

$$X|Y = A_j \sim N(\mu_j, \sigma).$$

The discriminant function

$$\delta_j(x) = x \cdot \frac{\mu_j}{\sigma^2} - \frac{\mu_j^2}{2\sigma^2} + \ln \pi_j$$

can be used to classify an observation by choosing the level A_j whose discriminant is largest at x.

We estimate the values of μ_i and σ from the sample data:

$$\hat{\mu}_j = \frac{1}{n_j} \sum_{i: y_i = A_k} x_i$$

$$\hat{\sigma}^2 = \frac{1}{n-\ell} \sum_{j=1}^{\ell} \sum_{i:y_i=A_k}^{\ell} (x_i - \hat{\mu}_j)^2$$

Simulated Data





Simulated Data





• What feature of the graph shows that $\pi_0 = .75$ and $\pi_1 = .25$?

Find Estimates

```
Estimates for \mu_j and \pi_j
d %>% group_by(Y) %>% summarize(pi = n()/n, mu = mean(X))
```

A tibble: 2 x 3
Y pi mu
<fct> <dbl> <dbl>
1 0 0.75 0.828
2 1 0.25 3.22

Find Estimates

```
Estimates for \mu_i and \pi_i
d %>% group_by(Y) %>% summarize(pi = n()/n, mu = mean(X))
## # A tibble: 2 x 3
##
    Y
          pi
                    mu
## <fct> <dbl> <dbl>
## 1 0 0.75 0.828
## 2 1
      0.25 3.22
Estimate for \sigma^2.
d %>% group_by(Y) %>% summarize(ssx = var(X) * (n() - 1)) %>%
  summarize(sigma_sq = sum(ssx)/(n-2))
## # A tibble: 1 x 1
##
     sigma_sq
##
        <dbl>
## 1 0.992
```

Solve for intersection of discriminant functions: $\delta_0(c) = \delta_1(c)$ when

Solve for intersection of discriminant functions: $\delta_0(c) = \delta_1(c)$ when

$$c = rac{\mu_0 + \mu_1}{2} + rac{\sigma^2(\ln \pi_0 - \ln \pi_1)}{\mu_1 - \mu_0}$$

Solve for intersection of discriminant functions: $\delta_0(c) = \delta_1(c)$ when

$$c = rac{\mu_0 + \mu_1}{2} + rac{\sigma^2(\ln \pi_0 - \ln \pi_1)}{\mu_1 - \mu_0}$$

c<- (mu0 + mu1)/2 + (sigma2*log(pi0) - log(pi1))/(mu1-mu0)
c</pre>

[1] 2.483001

Solve for intersection of discriminant functions: $\delta_0(c) = \delta_1(c)$ when

$$c = rac{\mu_0 + \mu_1}{2} + rac{\sigma^2(\ln \pi_0 - \ln \pi_1)}{\mu_1 - \mu_0}$$

c<- (mu0 + mu1)/2 + (sigma2*log(pi0) - log(pi1))/(mu1-mu0)
c</pre>

```
## [1] 2.483001
Write a function to create discriminant functions:
discriminant <- function(x, pi, mu, sigma2) {
    x * (mu/sigma2) - (mu<sup>2</sup>)/(2 * sigma2) + log(pi)
}
```

Solve for intersection of discriminant functions: $\delta_0(c) = \delta_1(c)$ when

$$c = rac{\mu_0 + \mu_1}{2} + rac{\sigma^2(\ln \pi_0 - \ln \pi_1)}{\mu_1 - \mu_0}$$

c<- (mu0 + mu1)/2 + (sigma2*log(pi0) - log(pi1))/(mu1-mu0)
c</pre>

```
## [1] 2.483001
Write a function to create discriminant functions:
discriminant <- function(x, pi, mu, sigma2) {
    x * (mu/sigma2) - (mu^2)/(2 * sigma2) + log(pi)
}</pre>
```

Evaluate discriminant function on data for each class:

```
d0 <- discriminant(d$X, pi0, mu0, sigma2)
d1 <- discriminant(d$X, pi1, mu1, sigma2)</pre>
```



Plots





Plots



• Why don't discriminant functions intersect at the same point as density curves?